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MODELING HIGH EXPLOSIVES WITH THE METHOD OF CELLS AND MORI-TANAKA EFFECTIVE MEDIUM THEORIES

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Submitted to:

MODELING HIGH EXPLOSIVES WITH THE METHOD OF CELLS AND MORI-TANAKA EFFECTIVE MEDIUM THEORIES

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Abstract. The Method of Cells (MOC) has been applied to a PBX 9501 composite, consisting of large explosive grains embedded in a small grain-binder mixture, to determine its thermal-mechanical properties. To treat the bimodal size distribution of grains, in the framework of the MOC, we assign one of eight MOC cells to model the effects of large grains and the remaining seven cells to model the small grain-binder mixture. We have applied a modified Mori-Tanaka effective medium theory to model the small grain-binder mixture. Spherical as well as randomly oriented ellipsoidal grains can be treated. This theory allows us to model the individual properties of the constituents: binder viscoelasticity, and grain elastic-plastic-damage behavior. Interfacial debonding between the grains and binder can be incorporated as needed. The method's predictions are compared to uniaxial measurements. [Research supported by the USDOE under contract W-7405-ENG-36.]

INTRODUCTION

The microstructure of PBX 9501 is very complicated because of the irregular size distribution of the cyclotetramethylene-tetranitramine (HMX) high explosive crystals in the PBX 9501 composite. It is tempting to use the powerful Method of Cells[1] (MOC) micromechanics to model this material. Because of the complex microstructure it appears that a large Representative Volume Element (RVE) is needed. Unfortunately, large RVE's become prohibitively expensive in computation time when implemented in finite-element simulations. To circumvent this problem, we propose to develop a hybrid theory where a small, numerically efficient, RVE accurately represents the entire PBX 9501 composite. This is done by using a portion of the RVE cells to represent the large HMX grains, while the remaining cells will consist of a mixture of small HMX grains and plasticized estane binder. This proposal eliminates the need to have RVE cells model HMX grains ranging from small (10 μm) to large (200 μm) sizes. The Eshelby-Mori-Tanaka (EMT) composite theory is used to determine the stress and strain fields in the mixture RVE cells, as described by Weng and coworkers[2]. The EMT theory includes rate-dependent polymeric materials because much of the rate dependence observed for PBX 9501 is due to the polymeric binder.

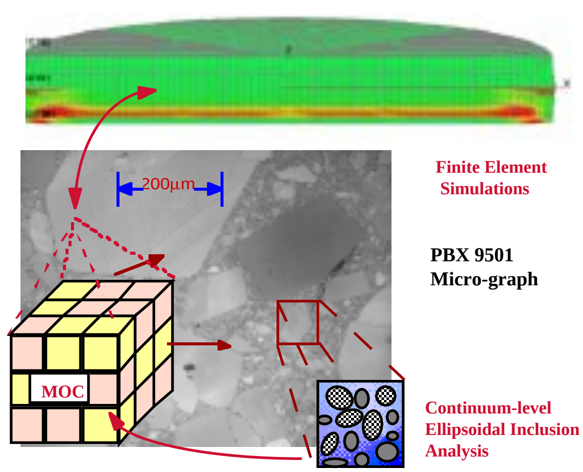

FIGURE 1. Treatment of the different length scales.

Figure 1 shows how we treat the various length scales in this problem. The cubical RVE has cells for coarse HMX grains and cells with small grain-binder mixture. The small grain-binder mixture is treated by EMT theory. Homogenization of the RVE in MOC theory allows the MOC/EMT theory to be implemented into large-scale finite element simulations. In this way we have bridged length scales from microns to centimeters.

THEORETICAL CONSIDERATIONS

A detailed discussion of the MOC has been given by Aboudi[1]; here we review only the qualitative details regarding the method. The MOC equations are derived from the following considerations: (1) volume averaged stress is continuous across cell boundaries, (2) volume averaged displacement is continuous across cell boundaries when interfacial bonding is perfect, (3) a first-order expansion suffices for the local particle displacement field, (4) conditions of mechanical equilibrium apply, (5) constitutive laws for the constituent materials are known, and (6) the micro-structure is spatially periodic (allowing the identification of a RVE). These conditions are sufficient to solve for the micro-stresses $\sigma_{ij}^{(\alpha,\beta,\gamma)}$ and micro-strains $\varepsilon_{ij}^{(\alpha,\beta,\gamma)}$ in the RVE cells. The macro-stress $\bar{\sigma}_{ij}$ for the entire composite system, for example, is determined from the weighted volume average of $\sigma_{ij}^{(\alpha,\beta,\gamma)}$ where α,β,γ labels the cells of the RVE.

We refer to the binder-HMX composite theory describing the mixture RVE cells as the Dirty Binder (DB) model (Fig. 2). In the DB model each mixture cell within the MOC scheme is a composite comprised of randomly spaced filler (f) HMX grains embedded in a matrix (m) of plasticized estane. Let the concentration of the HMX phase be denoted by c_f, and the plasticized estane by $c_m = 1 - c_f$. The grains are assumed to be randomly positioned in the matrix, and c_f is taken to be sufficiently small such that the probability of grain-to-grain contact is negligible (*e.g.* $c_f < 40\%$).

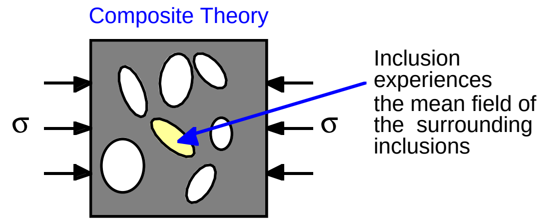

FIGURE 2. Dirty Binder Model using EMT Theory

The isotropic plasticized estane binder is viscoelastic and the HMX grains are treated as being linear elastic. The elastic moduli for HMX were taken from ultrasonic sound speed measurements of J. Zaug[3]. His Voigt upper bound values for the bulk and shear moduli are 12.51 GPa and 5.43 GPa, respectively, which are the values used in our calculations. The bulk modulus of the binder is taken to be 3.65 GPa. To describe the rate dependence of the shear relaxation function we developed a Generalized Maxwell Model (GMM) for the binder of the form:

$$\mu^m(t) = \sum_{i=1} \mu_i^m \, e^{-t/\tau_i}, \qquad (1)$$

where τ_i is the ith relaxation time and μ_i^m is the strength of the ith mode. The entire DB composite will respond viscoelastically, obtaining its strain rate dependence from the plasticized estane matrix. As with the plasticized estane, we expect that the Boltzmann Superposition Principle (BSP)[4] will provide an adequate description for the time dependent stress field, $\sigma_{ij}(t)$, for the entire DB composite,

$$\sigma_{ij}(t) = \int_0^t dt' \, L_{ijkl}^{DB}(t-t')\,\dot{\varepsilon}_{kl}(t'), \qquad (2)$$

where $L_{ijkl}^{DB}(t)$ is the stress relaxation function for the DB composite and $\dot{\varepsilon}(t)$ is the strain rate tensor. The random position of the HMX grains in the matrix ensures overall isotropy of the DB composite. Under these conditions $L_{ijkl}^{DB}(t)$ can be expressed as

$$L_{ijkl}^{DB}(t) = \left[K^{DB}(t) - \tfrac{2}{3}\mu^{DB}(t)\right]\delta_{ij}\delta_{kl} + \mu^{DB}(t)\left[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right], \quad (3)$$

where $K^{DB}(t)$ and $\mu^{DB}(t)$ are the DB composite bulk and shear relaxation functions, respectively. Our derivation of these two functions begins with the theory of Weng and coworkers[2]. These authors generalized Eshelby-Mori-Tanaka theory to include linear viscoelastic materials. Here we make no attempt to summarize the entire theory, rather we focus only on points central to our work. Each moduli, in EMT theory, has the form

$$\tilde{K}^{DB}(z) \equiv z\,\mathrm{L}\left\{K^{DBm}(t)\right\} = z\int_o^\infty dt\, e^{-zt}\, K^{DB}(t), \quad (4)$$

where L is the Laplace transformation operator.The HMX and the binder's bulk response are both approximated as being rate independent. Identifying the ratio $\tilde{\mu}^{DB}/K^{DB}$ as a small quantity allows us to expand the bracketed quantities in Eq. (4) in a power series about this ratio. The resulting expansions can be truncated to any order. This step is important because it allows us to perform analytic, rather than numerical, Laplace inversions required by Eq. (4) The result of our first-order analysis are the simple expressions

$$K^{DB}(t) = K_0^{DB} + \sum_{i=1}^{M} K_i^{DB}\, e^{-t/\tau_i} \quad (5)$$

$$\mu^{DB}(t) = \mu_0^{DB} + \sum_{i=1}^{M} \mu_i^{DB}\, e^{-t/\tau_i}, \quad (6)$$

$$K_i^{DB} = \begin{cases} K^f K^m (c_f K^m + c_m K^f)^{-1} & i = 0 \\ \frac{4}{3} c_f c_m (K^f - K^m)^2 \bullet (c_f K^m + c_m K^f)^{-2}\mu_i^m & i \neq 0 \end{cases}$$

$$\mu_i^{DB} = \begin{cases} 0 & i = 0 \\ (1 + \frac{5c_f}{2c_m})\mu_i^m & i \neq 0 \end{cases}$$

where μ_i^m are the coefficients of the GMM for the unfilled binder. This analysis has be extended to the general case of ellipsoidal shaped HMX grains.

COMPARISON WITH EXPERIMENT

Using our micromechanics theory we could simulate uniaxial compression experiments in regimes of low and intermediate strain rates. Accordingly, we were able to compare our theoretical stress-strain predictions for PBX 9501 to quasi-static MTS experiments done by Weigand[5] and Instron measurements of Idar, Peterson, Scott, and Funk[6]. At higher rates a similar comparison was made to Split Hopkinson Pressure Bar (SHPB) measurements of Blumenthal, Cady and Gray[7].

The DB model described in the last section can be incorporated into the MOC with relative ease. We then have seven DB cells and one large pure HMX cell forming the eight cells in the 2x2x2 RVE. Larger RVE's, for example 3x3x3 could be used in future calculations if the need arises. In the calculations described below only spherical HMX grains are used in the DB cells. From our simulations the optimal percent volume concentration of the HMX grains in the DB cells was determined to be about 40%.

The results are shown in Fig. 3 for various strain rates and temperatures. The temperature dependence in our theory comes completely from the temperature dependence of the binder using a Williams, Landel and Ferry (WLF) expression[4]. Regarding the theory-experiment comparison, three points need further comment. First, the change in the slope of the stress-strain curves, at low strains, comes about completely from the viscoelasticity of the binder. Second, there is substantial softening seen in all stress-strain curves beyond strains of about 1%. In our theory, this particular behavior was captured by using ISO-SCM crack model[8]. In our MOC/EMT hybrid theory only the pure HMX cell in our RVE was allowed to have micro-crack growth. Third, in SHPB experiments the initial portion of the curve is in question because of the required ring-up time for the sample. Nevertheless, good agreement between theory and experiment is generally found. Finally, we also compared our theoretical predictions to plate impact experiments of Dick, Martinez, and Hixson[9]. For this it was necessary to embed our micromechanics analysis into the finite-difference hydrocode. Our results were found to be in good agreement with those reported in Ref. (9).

CONCLUSIONS

We have applied Mori-Tanaka and Method of Cells composite theories to model the mechanical properties of PBX 9501. The method's predictions compare well to experimental measurements. Viscoelasticity of the binder[10] and elastic-plastic-damage properties of the HMX grains must all be accounted for to properly describe the behavior of this explosive.

ACKNOWLEDGMENTS

The authors gratefully acknowledge financial support for this work from the Joint DoD/DOE Munitions Technology Development Program and the (LANL) Laboratory.

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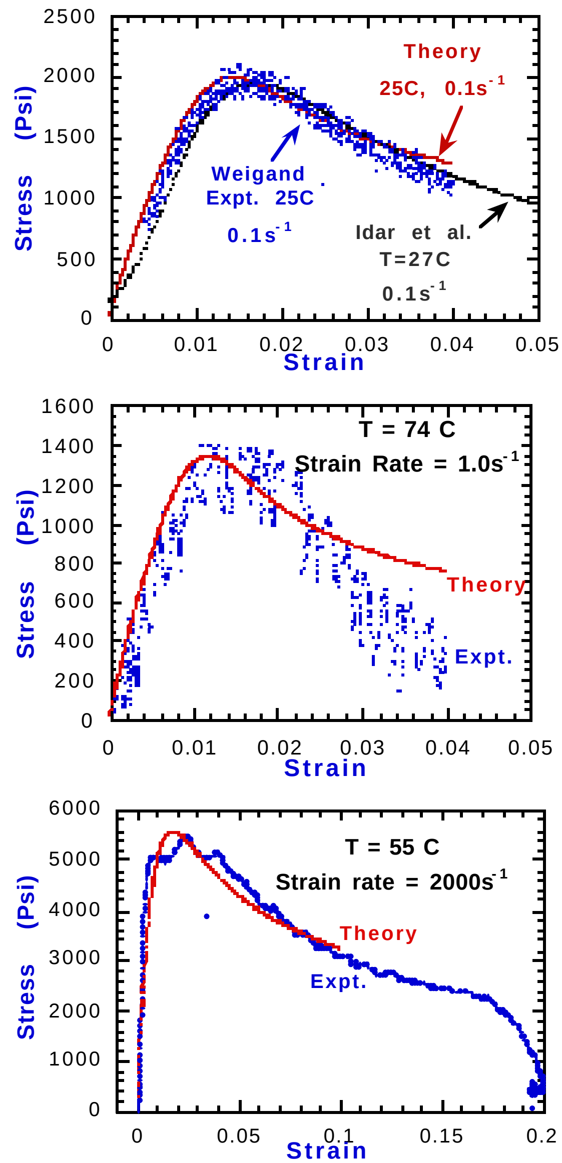

FIGURE 3. Low strain rate (top two) and high strain rate (bottom) comparisons between MOC/EMT theory and experiment.